ECE476: Electro-Optics
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Spectrophotometer Honors Option

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Abstract— This paper discusses an attempt to create a homemade spectrophotometer using a simple diffraction grating, a servo motor, a digital light sensor, an LED light source, a spectrometer sampling vile, other common household items (including cardboard, tape, and Legos), and some basic knowledge of light diffraction, geometry, and spectrometry. The goal of this experiment was to automate the otherwise manual process of developing a rough emission spectrum of various light sources, or absorption spectrum of various liquids. The light sources explored include a White LED, a Red LED, a red laser diode, and a White LED flashlight. The absorption spectrums that we will touch on include a spectrometer vial, pure water, salt water, and sugar water. We will also look at how dying water different colors affects the absorption spectrums of water. This paper will elaborate on the methods of creating our spectrophotometer system, as well as expand on some of the potential shortcomings of this experimental setup. Obviously, commercial spectrophotometers work extremely well, but here we propose a cheap alternative that can be both fun to make and useful to some degree.

Introduction

We start with a discussion of spectroscopy as a field of exploration. Spectroscopy is concerned with the absorption and emission of electromagnetic radiation, i.e., light, by atoms and molecules [1]. Spectroscopy has been a very useful tool of late in exploring and explaining concepts introduced by principles of quantum mechanics [1]. Spectroscopy is a useful tool in helping us to learn about and explore the things that are very small, such as the structures of individual atoms, but also very large things, such as the mysteries relating to our solar system! We can see that the scope of spectroscopy is therefore quite large. This paper will not go too in-depth about the theory of spectroscopy, but one super relevant concept relates to what we know about Schrödinger equation and the different energy levels of a substance. The specific wavelengths of light that that are absorbed by a substance are many times the same wavelengths that are emitted when electrons in the substance are excited to higher energy levels. This is just one example of an insight that spectroscopy can give into the properties of a substance. Infrared spectroscopy is another very useful tool, as it allows for the study of any material in virtually any state (solid, liquid, gas). It has also been used in the identification of different properties of different materials and categorizing different substances apart [2].

Our spectrophotometer presented here is made using a diffraction grating. Diffraction gratings are devices that take advantage of the wave-particle duality of light. When light passes through a single slit, the light waves constructively and destructively interfere to produce a pattern. A diffraction grating takes advantage of this idea and diffracts light in well-defined directions that are based on the wavelength of light incident on the device [3]. The relationship of angle of diffraction and wavelength is known as the grating equation, or the Bragg diffraction condition, and this equation will be broken down later in this report. This equation is what makes the diffraction grating specifically useful in spectroscopy, however. Diffraction gratings are still used in some modern-day spectrophotometers and understanding them in a general sense is essential to understanding the mechanics of a spectrometer and the principles of spectroscopy.

The following section will outline the methods used for designing a homemade spectrophotometer, as well as present the data for various experiments that were performed to prove the functionality of the spectrophotometer.

Methods, Data and Discussion

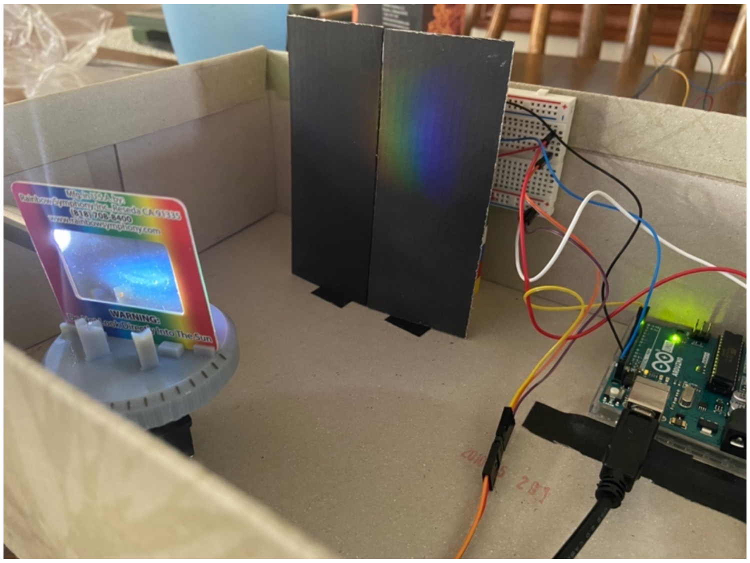

Figure 1: The experimental setup of the project.

We begin the methods section with discussion our spectrometer setup. We started with a carboard shoe box that will contain the entire spectrometer setup. Penetrating through the side of the box there is an LED light source that shines on a diffraction grating. This diffraction grating is mounted on top of a servo motor that will be connected to an Arduino for control. The diffraction grating was positioned so that the incident light will diffract into a small slit perpendicular to the servo motor. Behind this small slit there is a mount made from Legos that is used to hold the spectrometer vials that are used in this experiment. Behind that the light sensor can be found which is also connected to the Arduino to record values. Off to the top right of the board the Arduino is stored for convenience of wiring. Also, for wiring convenience, a bread board was mounted to the wall of the shoe box, as it was easiest to use a breadboard with double sided tape for temporary mounting and easy adjustment. This full setup can be seen in Figure 1 for easier visualizing.

We were able to take Arduino code for controlling a servo motor in 1-degree increments and merge that code with Arduino code for an Adafruit TSL2591 High Dynamic Range Digital Light Sensor. This Adafruit sensor, when configured with our Arduino, would give readings in Lux, and the Arduino made averaging and saving these readings both easy and convenient. Our method for coding our Arduino for use in our homemade spectrometer will follow.

We first made it so that the LED light shone perpendicular to our grating. This perpendicular angle was a good starting point and made it easy to make sure that the light and servo were physically positioned properly within the systems box. Next, the code set the servo to be 90 degrees to the LED. Following this, 5 readings were taken from the light sensor on 500 millisecond intervals, and these values were averaged. This average was then saved to the Arduinos memory and the servo motor was rotated 1-degree. The light sensor measuring, averaging, and saving process was then repeated followed again by a 1-degree rotation over 20 degrees, as this was an appropriate to capture an entire diffracted mode from the 1000 lines per millimeter diffraction grating. After all data was collected, the readings were printed to the Arduinos text log and then saved to the local computer that the Arduino was connected to. This allowed for the data to be analyzed.

The diffraction grating was 12.6 cm away from the slit that fed into the detector. Unfortunately, the servo motor did not seem to be very accurate in terms of its rotation angle when small changes to the angle were made. For example, an angle change of 25-degrees was measured over 20 1-degree increments. Therefore, it was decided that the starting angle and finishing angle were to be manually measured, and that linear increments over the 25-degree occurred. This is a reasonable assumption as the motor did appear to move with each increment, and the general trends in the data were consist over multiple measurement epochs for a single substance.

It is also important to note that because the sensor measured in the infrared, we decided to actually decrement the angle of incidence on the diffraction grating so that the red light will be incident on the sensor before the UV light, ensuring that infrared light was captured first in our readings.

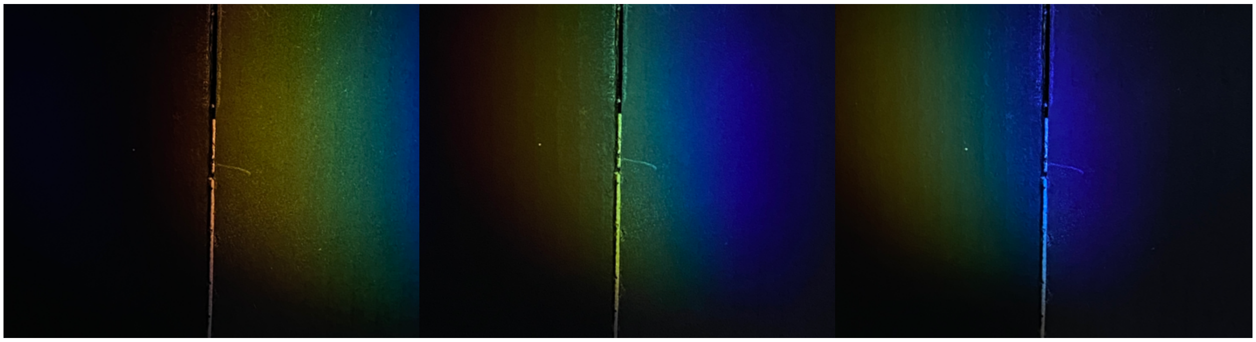

Figure 2: Proof of different wavelengths of light entering the slit and reflecting out

It was important to ensure that the incident light on the slit was in fact propagating through the slit and that the slit was properly sampling the desired wavelengths of light. This was verified, since we could see the desired wavelength of light reflecting out of the slit for various different wavelengths, as seen in Figure 2.

The measured sum of diffracted angle, and angle from diffracted angle to edge of the diffraction grating we will define as θ_s. This angle is used to derive the angles used in our calculations and it spanned, over 20 updates from 56° to 81°. This means that each increment followed a change in degrees of 1.25°.

We know that when the incident angle of light is not perpendicular to the diffraction grating, the following equation shows the relationship:

$$d\,[\sin(\theta_m) \pm \sin(\theta_i)] = m\lambda, \qquad m = 0, \pm 1, \pm 2, \ldots \tag{1}$$

In our case, we ensured that the sum of θ_i and θ_m of our experiment was always 90 degrees, as the location of the slit from the center of the diffraction grating never changed and we made sure that it was perpendicular to the grating at the start of our experiment.

With this information, we are able to take our 25-degree spread and solve for the θ_i and θ_m at each measurement. To do this, we solve for θ_i and θ_m with respect to θ_s.

We find that

$$\theta_i = 90^\circ - \theta_s$$

$$\theta_m = -180^\circ + \theta_s$$

Taking this and solving for equation 1 with respect to only θ_s, we find:

$$d\,[\sin(-180+)\ \pm\ \sin(90^\circ - \theta_s)] = m\lambda, \qquad m = 0, \pm 1, \pm 2, \ldots \tag{2}$$

We utilized mode -1 in our experiment, as it made the most sense given our setup, and it also appeared to be the brightest, hence, m = -1.

Knowing that we have a 1000 lines per millimeter diffraction grating, we solve for a slit width of d = 1µm. We now have everything that we need to know to solve for the wavelength of light that passed through our slit. Our computed wavelengths entering the small slit of our spectrometer can be found in the below Table 1. Note that the value for 81° is omitted as it wasn't recorded due to an oversight in the code.

θ_s°	Wavelength of transmitted light, λ (nm)
56	269.84
57.25	300.06
58.5	330.14
59.75	360.06
61	389.81
62.25	419.37
63.5	448.74
64.75	477.89
66	506.81
67.25	535.49
68.5	563.92
69.75	592.07
71	619.95
72.25	647.53
73.5	674.80
74.75	701.76

76	728.37
77.25	754.64
78.5	780.56
79.75	806.10
81	831.25

Table 1: Computed wavelength of transmitted light used in spectrometer readings.

Now that we know what wavelengths of light were entering into the small slit, we were then able to collect some data. We decided to develop first a spectrum for the white light from the LED. Next, we wanted to see the absorption of the spectrometer vile alone with the white light from the LED. We then collected the absorption spectrum data for this LED light propagating through the vile and plain water, sugar water, and salt water respectively. Finally, as our data was all based on the White LED flashlight, we collected the emission spectrums for various wavelengths.

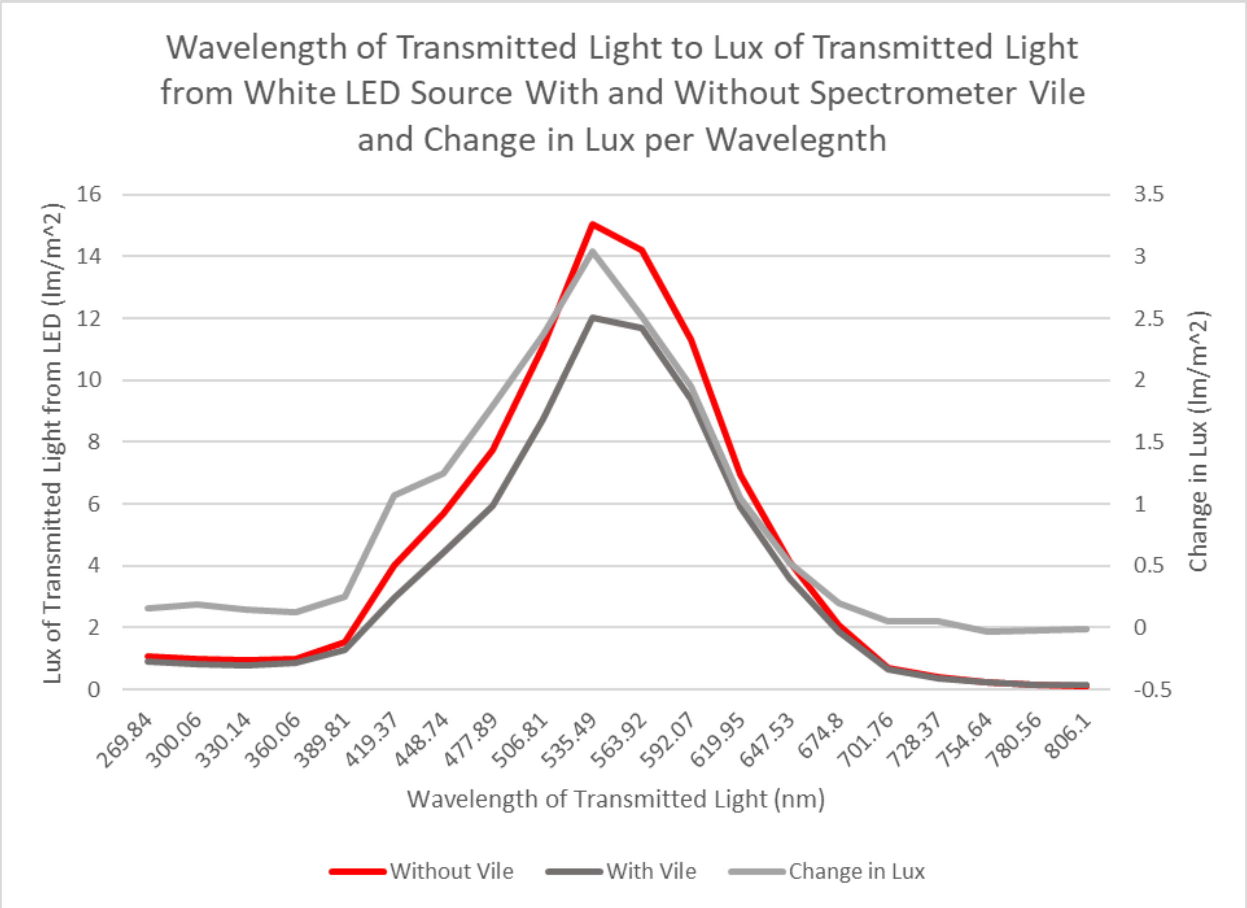

Figure 3: Change in lux of transmitted light with and without vile.

Starting with our first experiment where we measured emission spectrum alone in comparison to that emission spectrum propagating through the spectrometer vial, we can see the change in lux when we added the spectrometer vile in Figure 3. We notice that the change was not too significant, with the peak of change occurring relatively close to the peak lux wavelength for the light source. As all our substances must be held in the spectrometer vile, this is the data that will be compared against each substance to get an absorption spectrum of each liquid.

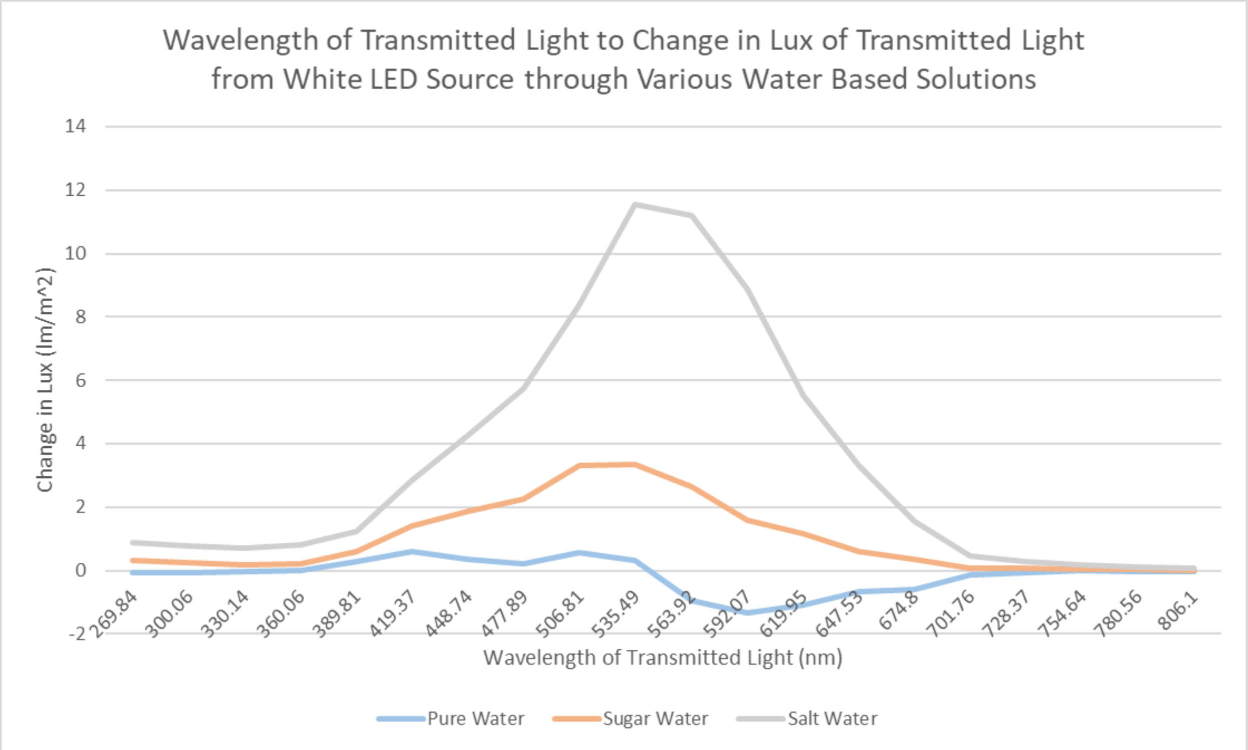

Figure 4: Change in lux of transmitted light through pure water, sugar water, and salt water.

In figure 4 we can see the change in lux of the transmitted light as it propagated through pure water, sugar water, and salt water. Here we subtracted the lux of the vile alone to observe these relationships. We can see that the light transmission through pure water did not change very much. Through sugar water it changed a bit more, and the largest change occurred in the salt water. This is most likely due to changes in concentrations of the different waters, as it has been shown that increasing the concentration of NaCl or Glucose in water decreases the spectroscopy of the substance. This is in fact one method to determine the concentration of NaCl or Glucose in a substance by its spectroscopy [4]. In this cited paper, this was achieved for much lower wavelengths, but it can be assumed that the same effect applies for shorter wavelengths as well. Looking at the overall trends of our data for sugar water, our graph does appear to reflect in curvature what would be expected for sugar water, validating our data [5].

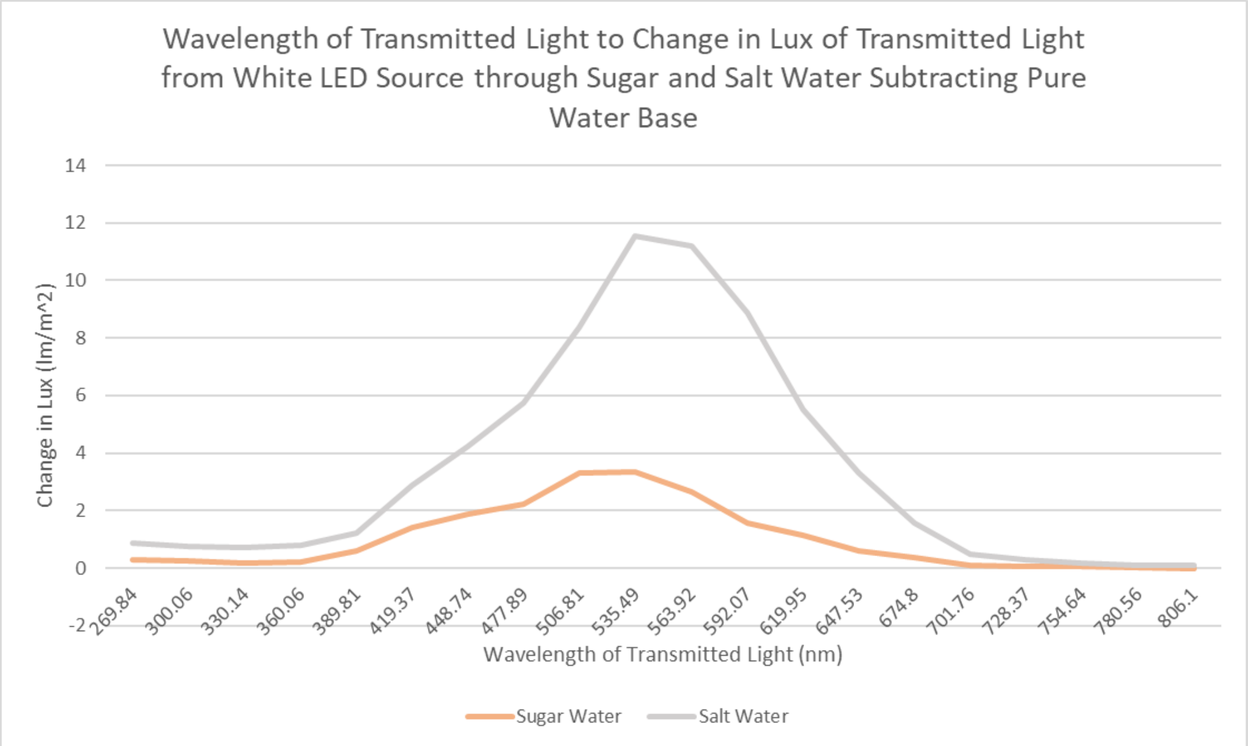

Figure 5: Change in lux of transmitted light through sugar and salt water, subtracting pure water.

Perhaps a more insightful graph can be found in Figure 5, where we can see the change in lux of the salt water and sugar water after subtracting the lux of the water alone. This allows us to see the impact of the salt and sugar alone, not accounting for the absorption of the pure water. In a sense, we are zeroing our spectrometer to see the influence that the salt and sugar alone has on the absorption spectrum. In our data here, we can see that the two have different peak wavelengths of absorptions. In theory, we should be able to use this absorption data to identify the substance in water if we were log the absorption spectrums of various different substances in water. This is a very simple example of how spectrometers are used in the real world to identify substances and the concentrations of substances in a liquid.

In an attempt to further verify our spectrometer, I thought it would be a good idea to see how different food colorings would affect the absorption spectra. We know that a substance of a certain color reflects light of that color, so we hypothesized that a red food coloring would reflect more red light, and a blue food coloring would reflect more blue light. We thought that this might lead to a visible difference when we collected an absorption spectrum from otherwise pure water.

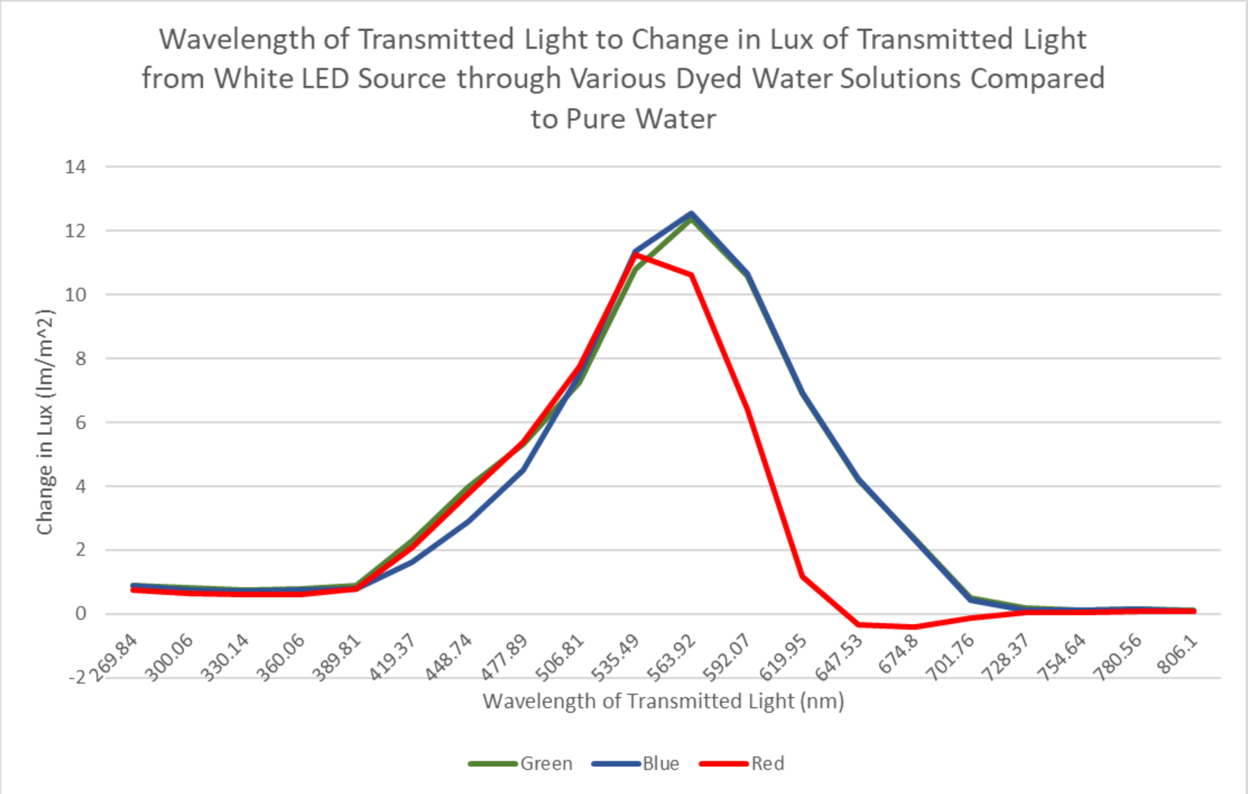

Figure 6: Change in lux of transmitted light through green, blue dyed water, red dyed water/

What we found can be seen in Figure 6. In this figure, we subtracted the lux pure water from each concentration to get the difference that the dyes caused. We see that the peak for the red vial is shifted to the left, away from the red wavelengths which supports our hypothesis. We also see that the peak for the blue light is at the higher wavelengths, also supporting our hypothesis. The green findings itself in the middle might go against what we thought would happen, but the fact that the peak for the green is slightly less than the blue could show that some green light is being reflected. Concentration can also play a significant role here, as well as the colors that we think we see not exactly corresponding with the wavelengths that we would expect, hence, we can say that our data is rather inconclusive.

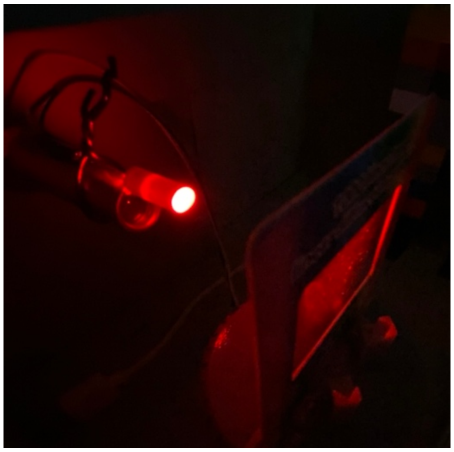

Figure 7: Example of a tube shaping the LED to focus the light and cut down on noise.

We really wanted to explore the different emissions spectrums of different light sources and we decided to use the White LED flashlight that we used for all the above experiments, as well as a Red LED, White LED, and Red Laser source. The LEDs were hard to concentrate the light onto the diffraction grating, so a tube was used to focus the light and prevent unwanted light from entering the sensor from reflections in the environment. An example of this can be seen in Figure 7. For the light sources, except for the White LED flashlight, the small slit was removed from within the sensor, as the light intensity was significantly less for the non-White LED flashlight sources, and we wanted to ensure that the light was being captured to a point where sensor noise became less relevant.

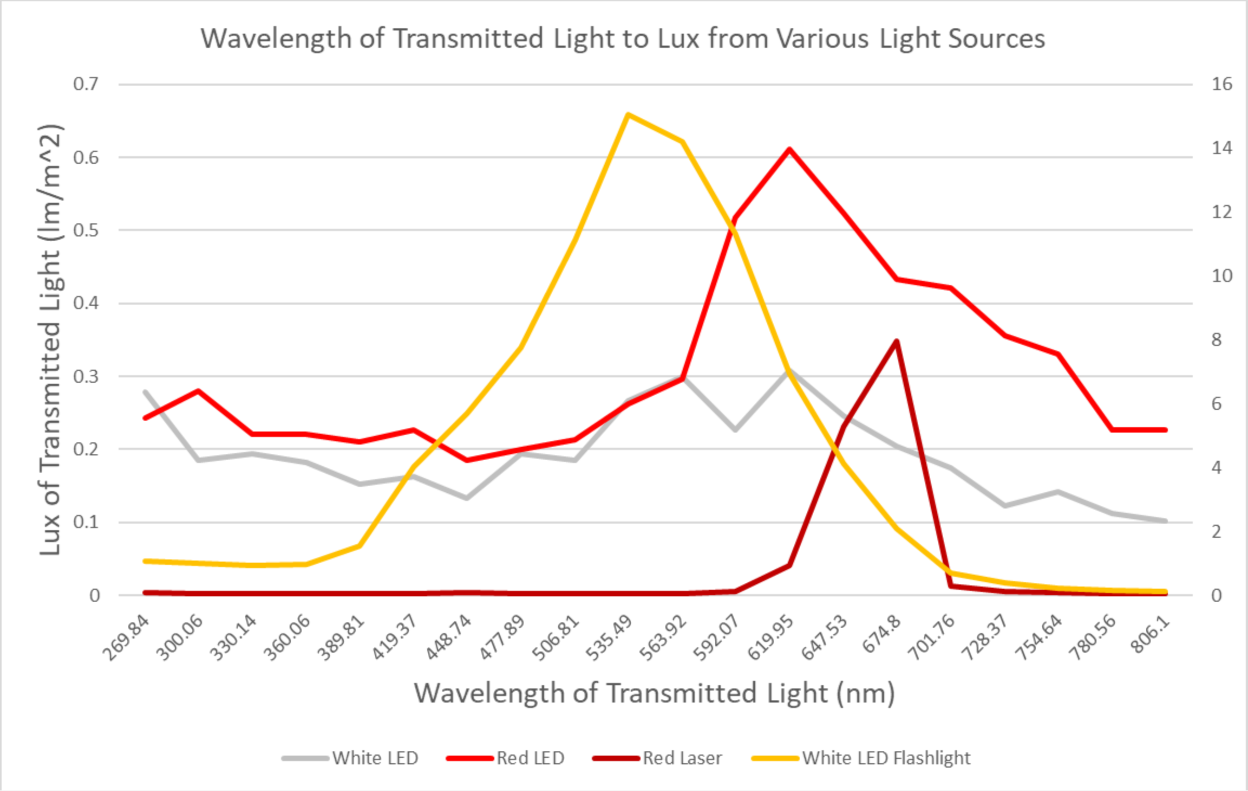

Figure 8: Collected emission spectrums of various LED sources

The emission spectrums corresponding to the lux of each source can be seen in Figure 8. We gain confidence in our spectrum and all our other data as the Red lase falls right into the category of red light. Its narrow beam also leads to a sharp peak in our graph which is encouraging. Our Red LED according to our measurements has a peak wavelength of around 620 nm. The data sheet for the Red LED lists its peak wavelength at 625 nm so we can see that our spectrometer absorption spectrum readings match well to what is expected [6]. Our White LED, which we would expect to have a trough at around 500 nm to combat human's sensitivity to green light, does not appear to have this trough on our graph, but the White LED also has the weakest lux of all 4 sources and perhaps there was an error in recording the data or an inability to focus the light well onto the diffraction grating and intern onto the sensor.

Analysis and Conclusion

Here we were successfully able to create a homemade spectrophotometer. Looking at the experimental data collected we can see how this spectrophotometer could be useful in some basic applications. This spectrophotometer can be useful tool in observing the general trend in emission wavelengths of any given light source, as well as the absorption spectrum of a liquid material.

Unfortunately, however, this spectrometer has some clear limitations. One major limitation is that the current setup does little to eliminate the role of ambient light in the system. The spectrometer must be used in a completely dark place, and even then, sometimes the reflected light from the light source itself can pollute the readings. This is most likely the reason that the observed curves in this report were so general; many readings were polluted by ambient light in the room. One solution to this would be to absorb unused light better. I also think that there can be a lot done to improve the efficiency of light emission from a source onto the light sensor. This can perhaps be achieved through some lenses to help narrow the light beams and direct it more precisely on the grating. I also think that perhaps propagating the light through an optical fiber might be a good idea to cut down on the ambient light. Propagating the light through an optical fiber and then running that fiber to a separate system would allow the sensor system to be fully isolated from the source, allowing us to greatly cut down on ambient light. Diffraction might be a limitation to this setup; however, I presume that we will be running a short enough cable where diffraction is not too relevant. Further investigation would be required to validate whether this idea would be helpful or not, but intuition says that it will be. Another limitation of this spectrometer is that there is most likely lots of error in general measurements and alignments. Much of this setup was “eyeballed” for accuracy, which means that many of the calculated wavelengths of light might be off to some degree. Furthermore, I believe that isolating a single mode from the diffraction grating through some filtering techniques might improve the accuracy of readings, as it is very possible that some of the infrared from the light one mode can pollute the UV light form another mode. It is also possible that the sensor used in this spectrometer was inaccurate or susceptible to noise, so that too might be an area of improvement if a more formal spectrophotometer system was to be developed.

In conclusion, we have been able to successfully demonstrate some rough emission spectrums of a White LED, a Red LED, a red laser diode, and a White LED flashlight with respect to the visible wavelengths of light. We were also able to demonstrate the absorption spectrums of a spectrometer vial, pure water, salt water, and sugar water, also with respect to the visible light spectrum. We demonstrated the how dying water affects the absorption spectrums, with the color of the dye being more reflected and more absorbed. Lastly, we discussed our findings on each, as well as elaborated on some improvements to our spectrophotometer system.

In the end, we can see the basic principles behind light diffraction can go a long way with respect to some of its applications. Here, we demonstrated more trivial experiments, but the systems and ideas presented here have tremendous applications across multiple fields including physics, chemistry, biology, and all fields that are any combination of the three.

We also saw how using some very simple and affordable materials, the ideas of spectroscopy can go a long way in developing a primitive spectrophotometer. For tasks that require very precise measurement, perhaps this system is too limited, but for more general applications, this simple spectrophotometer can work quite well.

References

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